

Propylbenzene
103-65-1 | DTXSID3042219

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 859 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.28e-01

Confidence level: 6.37e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propylbenzene</div> <div>Measured: 741</div> <div>Predicted: 859</div>	<div>Image not found</div> <div>Butylbenzene</div> <div>Measured: 2450</div> <div>Predicted: 1580</div>	<div>Image not found</div> <div>Ethylbenzene</div> <div>Measured: 170</div> <div>Predicted: 271</div>
<div>Image not found</div> <div>2,3,5-Trimethylphenol</div> <div>Measured: 4070</div> <div>Predicted: 345</div>	<div>Image not found</div> <div>Styrene</div> <div>Measured: 912</div> <div>Predicted: 358</div>	